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A Characterization and Evaluation of Coal Liquefaction Process Streams

Results of Inspection Tests on Nine Coal-Derived Distillation Cuts in the Jet Fuel Boiling Range

Topical Report

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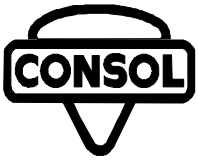

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ABSTRACT

This report describes the assessment of the physical and chemical properties of the jet fuel (180-300 °C) distillation fraction of nine direct coal liquefaction products and compares those properties to the corresponding specifications for aviation turbine fuels. These crude coal liquids were compared with finished fuel specifications specifically to learn what the refining requirements for these crudes will be to make them into finished fuels. The properties of the jet fuel fractions were shown in this work to require extensive hydrotreating to meet Jet A-1 specifications. However, these materials have a number of desirable qualities as feedstocks for the production of high energy-density jet fuels.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

Section 1
EXECUTIVE SUMMARY

The quality of the 180-300 °C distillation-fraction of nine direct coal liquefaction products was assessed by comparison of physical and chemical property test data to the corresponding specifications for aviation turbine fuels. Petroleum inspection tests were employed to evaluate the samples. Although it is acknowledged that these tests were not designed for analysis of coal liquids, they provide the best available methods for evaluation of the quality and value of the direct coal liquefaction product oils. In general, the coal-derived distillation fractions are too cyclic (aromatic, naphthenic) for use as commercial Jet A-1 aviation fuel and were shown in this work to require additional hydrotreating to meet Jet A-1 specifications. Instead of extensive hydrotreating, this fraction could be distributed in the refinery into the diesel fuel and gasoline feedstocks. However, its high volumetric energy content and compositional uniqueness (its naphthenic content, which makes the distillation cut unacceptable for Jet A-1), make this material a natural feedstock for high energy-density jet fuel. Although high energy-density fuels do not have potential to be a large part of the fuels market, but will be more a specialty product (albeit one with high value), continued research for the production of such fuels from coal under the auspices of the U.S. military is recommended.

Section 2
INTRODUCTION

The production of liquid fuels from coal via direct coal liquefaction technologies has been improved over the last two decades to produce high yields of high-quality coal-derived distillates. It may be more economically attractive to upgrade these distillates to transportation fuels in existing petroleum refineries as blends with petroleum feedstocks, rather than to construct grass-roots upgrading facilities designed specifically for coal liquids. Characterization of these liquids is a necessary first step to gaining admission of these products to the petroleum refineries. Once admitted to the refinery, correlations drawn between operating variables of the finishing process and net product oil characteristics (in regard to specification requirements) can be used to direct future coal liquid production efforts. Although it is acknowledged that the standard petroleum feedstock tests are not tailored for the analysis of coal liquids, it is believed that they are at least a starting point for this characterization. The comparison of the properties of the crude coal liquefaction products to specifications for finished fuels was made to determine what degree of refining the crude coal liquids must undergo once admitted to the refinery.

In support of the DOE direct coal liquefaction effort (under U.S. DOE Contract Nos. DE-AC22-89PC89883 and DE-AC22-94PC93054), net products and distillation cuts of those products from two modern, catalytic, integrated two-stage coal liquefaction facilities were collected and subjected to petroleum inspection tests. The products were acquired over a period of seven years from nine different tests at two different facilities. Three laboratories (IIT Research Institute, National Institute for Petroleum and Energy Research, Bartlesville, OK; Conoco Inc., Research and Engineering Dept., Ponca City, OK; and Inchcape Testing Services Caleb Brett Laboratory, Houston, TX) each applied petroleum inspection tests to two or more of the direct coal-liquefaction process-derived net product oils and the distillation cuts of the net product oils.

The distillations of the crude products and analyses of the net products and the distillation cuts were done at different times throughout the seven-year period by the different analytical laboratories. Not all tests were requested for all samples. However, all the net products were distilled to cut points which allowed the cuts to be grouped in general classifications. These

classifications were used to compare them to traditional petroleum refinery products. These classifications were: naphtha (IBP - ca. 190 °C), light distillate (also called kerosene or jet fuel, ca. 180-300 °C) heavy distillate (ca. 300 - 340°C), and resid (>340°C). The following report deals with the light distillate (ca. 180-300 °C) and its potential as a feedstock for jet fuels.

Reports and several presentations describing the results of the analyses for each net product oil and its distillation cuts were published previously.[1-16] This report is a compilation made of all the data specific to the jet fuel distillation cut. The range of feedstocks and production conditions validates the results presented here as being representative of modern two-stage coal liquefaction net products, and provides a comprehensive overview of the potential of these materials as refinery feedstocks and high-energy density jet fuel sources.

Section 3
EXPERIMENTAL

Brief summaries of the tests under which the net product oils were produced are provided below and in Table 1. Feed coals included bituminous coal from the Pittsburgh and Illinois No. 6 seams and subbituminous coal from the Wyodak and Anderson seam. In addition, one feed was a 50:50 mixture of Illinois No. 6 coal and a petroleum resid (Hondo vacuum tower bottoms). Reactor temperature sequencing for the two-stage liquefaction tests included both high/low and low/high configurations. All tests, with the exception of Runs 260D and CC-15, were made with catalyst in both reactors. Supported catalysts were used in Runs 259, 260, CC-15, CMSL-2, POC-1, and POC-2. Dispersed slurry catalyst was used in Runs PBO3 and PBO5. Table 1 also indicates which laboratory analyzed the sample and the corresponding distillation cuts.

Table 2 shows the distillation cuts which were produced from the net products and the equivalent petroleum cut designation. The samples were not all distilled to the same cut points. In several cases, multiple cuts comprise the jet fuel cut.

The yield of jet fuel fractions, expressed as volume and weight percent of the crude oils, are provided in Table 4. With the exception of the sample from Run 260D, the jet fuel fraction for the samples comprises on average 35-40 wt % of the crude oils. The yield of jet fuel on an MAF coal feed basis can be calculated from the elementally balanced process streams which were combined to produce the net crude product oil. These data were used to calculate the net product oil yield for Wilsonville Run 259G.[34] The net product oil yield was 73.02 g/100 g MAF coal. Thus, the jet fuel fraction from Run 259G comprises 22.9 g/100 g MAF coal.

The methods used to analyze and test the jet fuel cuts are provided in Table 3. Several of the measurements were obtained using different methods for different samples; these are designated on Table 3 as Method A, Method B, etc. When different methods were used to obtain the same measurement, the test used is indicated in the table of results (Table 4) by a superscript A, B, etc., referring to Method A, Method B, etc. Methods for gas chromatography/

mass spectrometry (GC/MS), ^{1}H-NMR spectrometry, and phenolic -OH determinations by Fourier transform infrared (FTIR) spectroscopy are provided in References 17-21.

Several of the jet fuel cuts were caustic washed. The procedure is provided in Reference 7. Analyses of the original jet fuel cut and the caustic-washed raffinate are provided in Table 5. None of the materials shown in Table 4 were caustic washed.

Section 4
RESULTS AND DISCUSSION

The major findings from the analyses of the jet fuel cuts of nine direct coal-liquefaction net products are described below. A brief description of the processing run for each sample is provided. Details of the runs can be found in the references. Some comparisons are made among the different samples; however, the emphasis of this report is the comparison of the coal-derived jet fuels and the ASTM or U.S. military specifications for jet fuels (Jet A-1, Jet B, JP 8 (the military equivalent of Jet A-1) and a potential application as a high energy density jet fuel. The specifications for Jet A-1 are provided on Table 4. Comparisons with other jet fuel specifications are provided in the following discussion.

PROCESSING RUN DESCRIPTIONS

Wilsonville Run 259G[22]

The major objectives of Wilsonville Run 259 were to investigate the maximum distillate yield while processing deep-cleaned Pittsburgh seam coal in the catalytic/catalytic mode of operation, to obtain a better-defined boiling end point for the distillation, to compare the performance of Ireland Mine Pittsburgh Seam coal with that of Illinois No.6 coal, and to test coals of different ash contents. Period G, in operation from April 30 through May 4, 1990, used deep-cleaned Ireland Mine coal and Shell 324 catalyst in both reactors, with a catalyst replacement rate of 2 g/kg MF coal. A forty-liter sample of net product distillate was obtained during period G for analyses.

Wilsonville Run 260D[23]

Run 260 was made between August 1990 and November 1990. The primary objective of Run 260 was to improve distillate yield with low-rank coal. The feed coal was Black Thunder Mine, subbituminous coal from the Wyodak and Anderson seam. Period D was a three day period from October 7-10. During period D, the reactors were configured catalytic/thermal, high/low (temperature sequence). The catalyst used was 1/16-inch extrudate of Shell 324 (Ni/Mo on Alumina). The interstage separator was not used in period D. Therefore, all first-stage products were sent to the second stage. The crude product from Run 260D was contaminated with Dowtherm A. The components of this heat transfer fluid (biphenyl and diphenyl ether)

interfere with the results of many of the analyses. A 9 L sample of crude product was distilled. This produced an insufficient amount of jet fuel fraction for all of the analyses. An additional 7 L was distilled and the jet fuel fractions from the two distillations were blended before testing.

HRI Bench Unit Run CC-15[24]

The objective of HRI's CTSL Run CC-15, also called Run 227-75, was to test a predispersed (impregnated) hydrated iron oxide catalyst. The feed coal was Wyodak and Anderson seam, Black Thunder Mine, subbituminous coal. Start-up and make-up oil for Run CC-15 was filtered process-derived liquid, produced in HRI Run 260-03, which also used Black Thunder Mine coal. Throughout Run CC-15, the first stage reactor was operated thermally; Shell S-317 Ni/Mo on alumina catalyst was present in the second-stage reactor. No in-line hydrotreater was used in the run. The net product sample was produced by compositing a total of 26 sample aliquots obtained during the run from the Separator Overhead (SOH) process stream and the Atmospheric Still Overhead (ASOH) process stream. A total of 16.5 kg of SOH and 6.9 kg of ASOH was blended and distilled

HRI Bench Unit Run CMSL-2[25]

The main objective of HRI's Run CMSL-2, also called Run 227-78, was to investigate the effect of a high coal concentration on process performance. In this continuous two-stage liquefaction run, the high coal concentration in the coal-solvent slurries was accomplished by lowering the solvent-to-coal ratio from 1.2 (to as high as 1.6) used in previous bench-scale runs, to 0.9 in CMSL-2. The feed coal was Illinois No.6, Burning Star 2, bituminous coal. Throughout Run CMSL-2, the first- and second-stage reactors were operated catalytically; Shell S-317 Ni/Mo on alumina catalyst was present in both reactors. No in-line hydrotreater was used in the run. The net product sample was produced by compositing a total of 10, 2 L sample aliquots obtained during periods 8 through 12 of the run from the Separator Overhead process stream and the Atmospheric Still Overhead process stream.

HTI Proof-of-Concept Run POC-1[26]

HTI Run POC-1 (also known as Run 260-04) was conducted October 1993 though February 1994. The main objective of the run was to scale up the CTSL process with Illinois No. 6 coal in the extinction recycle mode to produce an all-distillate product slate. The reactor

configuration was catalytic/catalytic with low/high reactor temperature sequence. AKZO AO60 (Ni/Mo on alumina, 1/16") catalyst was used in both stages. The in-line hydrotreater was employed, but it did not operate effectively during the run. Twenty-four liters of net distillate product were obtained for testing.

HTI Proof-of-Concept Run POC-2[26]

The main objective of Run POC-2, conducted in June and July 1994, was to scale up the CSTL process in the extinction recycle mode with subbituminous coal. An on-line hydrotreating unit was operational for the run. Although plastics and rubber were processed with coal during part of this run, the process oils described here were obtained from coal-only conditions. The run was operated in a low/high reactor temperature sequence. The catalyst used to charge the reactors was the spent catalyst from Run POC-1. Catalyst replacement rates were 1-1.5 lb/ton MF coal and 2-2.5 lb/ton MF coal in reactors 1 and 2, respectively. Twenty-four liters of net distillate product were obtained for testing.

HTI Bench Unit Run PBO3-6,7,8[27]

The bench unit Run PBO3 was conducted over 32 days in March and April of 1996. The primary objective of the run was to test different types and amounts of dispersed slurry catalyst. The effect of hydrotreatment of the recycle solvent on overall process performance also was investigated. The feed coal for the entire run was Black Thunder Mine, subbituminous coal. Reactor temperature sequence was low/high. The sample was collected during Periods 6, 7, and 8 (one 24 h day, each period) of Condition 2. In Condition 2, a dispersed iron/molybdenum catalyst was used. The samples were processed through the in-line hydrotreater. A total of 10.0 kg of sample blended from periods 6-8 was distilled.

HTI Bench Unit Run PBO3-9,10,11[27]

This is the second sample obtained from Run PB03 (see above). Periods 9, 10, and 11 make up Condition 3 of Run PBO3. The catalyst ratio in Condition 3 was 20/1 iron/molybdenum. This differed from Condition 2 (periods 6, 7, and 8), in which the ratio of iron/molybdenum was 10/1. The hydrotreater was bypassed in Condition 3. Other conditions were essentially unchanged from Condition 2. An 8.80 kg sample blended from periods 9-11 separator overhead samples was submitted for distillation.

HTI Bench Unit Run PBO5-22-25[28]

Run PBO5 was conducted from August 11 through September 1, 1996. Periods 22-25 (Condition 6) were the last 4 days of the run. A dispersed catalyst composed of iron, molybdenum, and phosphorus (10:5:1 ratio) was used. The feed composition for Condition 6 was 50% Crown II Mine, Illinois No. 6 bituminous coal, and 50% Hondo vacuum tower bottoms oil. The in-line hydrotreater was not used during this run condition. A 10.9 kg sample of separator overhead oil (blended from periods 22-25) was obtained for testing.

PROPERTIES IN COMPARISON TO JET A-1 SPECIFICATIONS

As was explained above, the jet fuel cuts from the nine different oils have different boiling ranges (Table 4). The overall temperature range of the cuts is 177-288 °C. With the exception of the 193-266 °C cut for Run 260D, the jet fuel range materials comprise ca. 30 to 45 wt % of the crude oil. Although only a "heart cut" of this material would probably be directed in a refinery to a jet fuel product, this represents a substantial yield of jet fuel. On this basis alone, jet fuels could be major end-products from direct coal liquefaction. Some of the samples were hydrotreated with in-line hydrotreaters, others were not (see run descriptions, above). This becomes significant in interpreting the properties, as described below.

The sulfur and mercaptan sulfur contents for most of the samples meet or exceed the Jet A-1 specification (Jet B has the same specification). One exception is the product from Run PBO5, in which Hondo vacuum resid was coprocessed with coal. The Hondo resid, which was 50% of the feed, contained 4.39 wt % sulfur. This elevated the jet fuel cut sulfur content. The processing of the coal liquid distillate through a hydrotreater has an evident effect on the sulfur content. This is demonstrated in the case of two samples produced under the same conditions with the primary exception that an in-line hydrotreater operated (PBO3-6, 7, 8) or did not operate (PBO3-9, 10, 11). In the case in which the hydrotreater operated, the sulfur content is much lower. Thus, the sulfur content in the crude coal-derived oils can be substantially reduced by hydrotreating oils. This could be accomplished, as with the sample from PBO3-6, 7, 8, in the coal-liquefaction plant or deferred to a downstream refinery.

The low-temperature behavior of the samples (the freeze point) is generally within 10 °C of the Jet A-1 specification (-40 °C, max) and in many samples meets the Jet B specification (-50 °C,

max). The copper strip corrosion properties meet Jet A-1 specifications for all samples, with the exception of two (PBO3-6, 7, 8 (204-288 °C) and PBO3-9, 10, 11 (177-204 °C)). Flash points meet specification (38 °C, min) for all samples. The viscosities of the samples are close to the specification of 8 cSt maximum at -20 °C for Jet A-1, with one (perhaps questionable) exception (Run PBO3-9, 10, 11 (204-288 °C cut)). The low-temperature viscosity of the sample from Run 260D and Run PB-05 (204-288 °C) also is greater than most of the other samples. However, even for these samples, it can be seen that careful blending of the different distillation cuts within the jet fuel boiling range can produce feedstocks with Jet A-1 specification viscosity.

Stability to auto-oxidation and polymerization at the operating temperatures is measured as a "thermal stability" measurement. These measurements are related to the amount of deposits formed in the engine fuel system on heating the fuel. The test uses the jet fuel thermal oxidation tester (JFTOT)[29]. All samples failed the JFTOT test, likely due to the high olefins and phenolics contents, which can have a detrimental effect on thermal stability.

Most samples did not meet the Jet A-1 or Jet B specification (7 mg/100 mL) for existent gum (the amount of material remaining on vaporization of the sample). Notable in exception were the samples from HTI Run POC-2 and PBO3-6, 7, 8. Olefins can be instrumental in the formation of gums; the HTI POC-2 product has a low olefins content. The operation of the hydrotreater during PBO3-6, 7, 8 may explain why that product also has low existent gum values.

The samples all have lower hydrogen contents (10.2-13.2 wt %) than petroleum derived jet fuels (13.5-14.0 wt %). This is related to the high aromatics content of the samples, which are in the range of 21.1-60.7 wt %. Only one cut of the Run POC-1 product meets ASTM specifications for Jet A-1 aromatics (25 vol % max). As a result of the high aromaticities, none of the samples meets the smoke point specification for Jet A-1 and Jet B. Also, the aromatic and naphthenic contents of the samples are responsible for the API gravity of all samples being lower than the Jet A-1 specification. Hydrotreatment of the samples to reduce the aromaticity will increase the hydrogen contents and improve the smoke points and API gravities. Either by hydrogenation or by hydrocracking, the aromatic contents of coal-derived jet fuels can be

reduced. Surprisingly, both methods under the right conditions produce materials that meet ASTM specifications.[30] All samples failed to meet the specification for luminometer number. This value is a measurement of the radiation emitted and the temperature rise in a flame. It is related to the hydrocarbon-type composition of the fuel. Hydrotreating the coal-derived distillates also would improve this specification.

The heat of combustion on a MJ/kg basis is lower for all the samples than the Jet A-1 specification (which is the same for Jet B). However, on a volumetric energy density basis (MJ/L), all the coal-derived jet fuels meet or exceed the Jet A-1 specification (Table 6). This characteristic may make these materials desirable feedstocks for the manufacture of high energy density jet fuels.

The desirable property of high energy-density jet fuels is to pack more energy into a smaller volume. This results in extending the range of the aircraft. In addition, jet fuel is the primary coolant used to cool both the aircraft engine and the aircraft fuselage. To provide the necessary cooling, the fuel must be able to absorb approximately 3.5 MJ/kg and not break down under pyrolytic and auto-oxidative conditions.[32] Naphthenic fuels (especially polycyclic naphthenics) have been found to be good candidates for high energy-density jet fuels because they undergo endothermic reaction and contain high volumetric energy contents.[31] The volumetric energy content (Btu/gal) of polycyclic naphthenes is, on average, 16% greater than commercial jet fuels.[31] Thus, the unique high-naphthene content of coal-derived jet fuels may make them attractive sources of high energy-density jet fuels. Petroleum-derived jet fuels can not easily be modified to improve this important property; thus, this may be a niche application for coal-derived jet fuels. This concept should be further explored.

CAUSTIC WASHING

The presence of phenolics in the jet fuels is undesirable. The phenolics were removed from several of the jet fuel cuts by caustic washing. Analyses of the jet fuel cuts and the raffinates are provided in Table 5. Caustic washing resulted in a significant reduction of the mercaptan sulfur content, in addition to phenolics. Other properties improved slightly. However, there was a decrease in the oxidation stability in the CMSL-2 sample. It is believed that this is a result of

the removal of hindered phenols which are known antioxidants.[7] Removal of the undesirable phenolics by caustic washing, although effective, results in loss of hydrocarbon product.

ADDITIONAL ANALYSES

Gas chromatography/mass spectrometry (GC/MS), determination of the phenolic -OH content, and ^{1}H-NMR spectroscopy of several of the samples were completed at the CONSOL R&D facility in Library, PA. These results are in addition to those obtained from the three laboratories which provided the petroleum inspection test results.

The total ion chromatogram for the jet fuel cut of Run 259G product is shown in Figure 1. Identifications of the prominent peaks are provided in a key immediately following the figure. The predominant cyclic nature (naphthenic, aromatic, hydroaromatic) of the components of these materials is apparent; virtually none of the major peaks are normal or branched paraffins. The total ion chromatogram for the jet fuel cut of Run 260D is shown in Figure 2. A comparison of it to the chromatogram for Run 259G jet fuel shows that the product of the subbituminous coal has a greater concentration of normal paraffins, olefins, and phenols. The crude from Run 260D was contaminated with Dowtherm A. The components of this heat transfer fluid (biphenyl and diphenyl ether) are apparent in the chromatogram.

The phenolic -OH concentrations and the phenolic and total oxygen contents of the jet fuel fractions are provided in Table 4. The phenolic oxygen content is calculated from the determined phenolic -OH concentration. The total oxygen content is a by-difference value from the analyses provided in Table 4. The phenolics tend to concentrate in the jet fuel fraction because of their boiling points. This was observed previously by other workers[3] with different coal-derived syncrudes. The phenolic -OH content of the Run 260D jet fuel is 3.7 times greater than that of the Run 259G products. The Run 260D total oxygen content also is much higher than the Run 259G products. However, Dowtherm A contamination is likely responsible for the much higher oxygen in the Run 260D jet fuel cut. The HTI CC-15 and CMSL-2 jet fuel cuts contain substantially less total oxygen than the Run 259G and Run 260D materials.

Proton distributions were obtained for the jet fuel cuts of Wilsonville Runs 259G, 260D, HTI Runs CC-15, and CMSL-2. The data are included in Table 4. The contamination by Dow-

therm A in the Run 260D sample is evident in the lower than expected hydrogen content (10.6 wt % for Run 260D versus 11.5 wt % for Run 259G) and the higher than expected aromatic hydrogen content (17.0% versus 8.8 % for Run 259G). The aromatic hydrogen content for Run CC-15 product is similar to Wilsonville Run 259G product. The CMSL-2 samples, however, contain less (6.8% and 6.3%) aromatic hydrogen and more paraffinic (alkyl beta plus gamma) hydrogen. This is a result of the different feed coals; subbituminous coal produces more paraffins.

Section 5

REFERENCES

1. Kramer, R. L. "Modified Light Oil, Southern Clean Fuels Inc. - Coal Liquefaction Material, Sample Number C9034, Research Report" in "Coal Liquefaction Process Stream Characterization and Evaluation, Technical Progress Report, October 1 through December 31, 1990", DOE/PC 89883-24, June 1991.

2. Kramer, R. L. "Modified Light Oil, Southern Clean Fuels Inc. - Coal Liquefaction Material, Sample Number C90116, Research Report" in "Coal Liquefaction Process Stream Characterization and Evaluation, Technical Progress Report, July 1 through September 30, 1991", DOE/PC 89883-34, November 1991.

3. Brandes, S. D.; Winschel, R. A.; Burke, F. P.; Robbins, G. A "Coal Liquefaction Process Streams Characterization and Evaluation, Technical Progress Report, January 1 through March 31, 1991", DOE/PC 89883-27, September 1991.

4. Robbins, G. A; Brandes, S. D.; Winschel, R. A.; Burke, F. P. "Coal Liquefaction Process Streams Characterization and Evaluation, Technical Progress Report, October 1 through December 31, 1991", DOE/PC 89883-43, March 1992.

5. Zhou, P.-Z.; Marano, J. J.; Winschel, R. A. "Strategic Considerations of Coal Liquid Refining", *Am. Chem. Soc. Div. Fuel Chem. Prepr.* **1992**, *37*(4), 1847.

6. Robbins, G. A; Brandes, S. D.; Winschel, R. A.; Burke, F. P. "Coal Liquefaction Process Streams Characterization and Evaluation, Technical Progress Report, July 1 through September 30, 1993", DOE/PC 89883-86, March 1994.

7. Sturm, G. P.; Kim, J.; Shay, J. "Coal Liquefaction Process Streams Characterization and Evaluation, Topical Report", DOE/PC 89883-92, January 1994.

8. Robbins, G. A; Brandes, S. D.; Winschel, R. A.; Burke, F. P. "A Characterization and Evaluation of Coal Liquefaction Process Streams, Technical Progress Report, June 29 through September 30, 1994", DOE/PC 93054-4, October 1994.

9. Cabbiness, D. "Light Oil Assay of C95029, Syn Products of CONSOL, Technical Service Report" in "A Characterization and Evaluation of Coal Liquefaction Process Streams, Technical Progress Report, July 1 through September 30, 1995", DOE/PC 93054-20, December 1995.

9a. Cabbiness, D. "Light Oil Assay of C95028, Syn Products of CONSOL, Technical Service Report" in "A Characterization and Evaluation of Coal Liquefaction Process Streams, Technical Progress Report, July 1 through September 30, 1995", DOE/PC 93054-20, December 1995.

10. Robbins, G. A; Brandes, S. D.; Winschel, R. A. "A Characterization and Evaluation of Coal Liquefaction Process Streams, Technical Progress Report, July 1 through September 30, 1996", DOE/PC 93054-41, August 1997.

11. Kelly, R. "Crude Assay on HTI PBO3-6,7,8" in "A Characterization and Evaluation of Coal Liquefaction Process Streams, Technical Progress Report, July 1 through September 30, 1996", DOE/PC 93054-41, August 1997.

11a. Kelly, R. "Crude Assay on HTI PBO3-9,10,11" in "A Characterization and Evaluation of Coal Liquefaction Process Streams, Technical Progress Report, July 1 through September 30, 1996", DOE/PC 93054-41, August 1997.

12. Hughes, S. "Laboratory Report No. 97-000431-0-Hous;1" in Kelly, Robert "Crude Assay on HTI PBO3-6,7,8" in "A Characterization and Evaluation of Coal Liquefaction Process Streams, Technical Progress Report, July 1 through September 30, 1996", DOE/PC 93054-41, August 1997.

13. Winschel, R. A. "Inspection of Net Products of HTI Runs POC-1 and POC-2" presented at the Refining and End Use Review Meeting, San Antonio, TX, November 14, 1995.

14. Zhou, P.-Z.; Winschel, R. A.; Klunder, E. B. "Premium Distillate Products from Direct Liquefaction of Coal", *Am. Chem. Soc. Div. Fuel Chem. Prepr.* **1994**, *39*(4), 1204.

15. Winschel, R. A.; Zhou, P.-Z. "Inspection of Integrated Two-Stage Liquefaction Products by Petroleum Assay" presented at the Sixteenth Annual EPRI Fuel Science Conference, Palo Alto, CA, June 18-20, 1991.

16. Zhou, P.-Z. "Characterization of Coal/Resid Coprocessing Liquid Product (HTI Run PB-05)" DOE/PC92100, Subtask 44.01, May 1997.

17. Winschel, R. A.; Robbins, G. A.; Burke, F. P. "Coal Liquefaction Process Solvent Characterization and Evaluation, Technical Progress Report, July 1985 through September 1985", DOE/PC 70018-13, December 1985.

18. Burke, F. P.; Winschel R. A.; Pochapsky, T. C. "Composition and Process Performance of Distillate Recycle Solvents from the SRC-I Process", *Fuel* **1981**, *60*, 562.

19. Winschel, R. A.; Robbins, G. A.; Burke, F. P. "Correlation of Microautoclave and ^{1}H-NMR Measurements of Coal Liquefaction Solvent Quality", *Fuel* **1986**, *65*, 526.

20. Winschel, R. A.; Robbins, G. A.; Burke, F. P. "Phenolic -OH as a Process- Performance Indicator in Two-Stage Liquefaction", *Am. Chem. Soc. Div. Fuel Chem. Prepr.* **1985**, *30*(4), 155.

21. Burke, F. P.; Winschel, R. A.; Robbins, G. A. "Recycle Slurry Oil Characterization Final Report October 1980 - March 1985", DOE/PC 30027-61, March 1985.

22. Southern Clean Fuels, Wilsonville Advance Coal Liquefaction R&D Facility, Handouts from Technical Meetings No. 103 (March 14, 1990), and No. 104 (May 16, 1990) and No. 105 (July 11, 1990).

23. Southern Clean Fuels, Wilsonville Advance Coal Liquefaction R&D Facility, Handouts from Technical Meetings No. 106 (September 19-20, 1990), and No. 107 (November 14-15, 1990) and No. 108 (January 17, 1991).

24. Lee, T. L.; Comolli, A. G.; Johanson, E.; Stalzer, R. "A Study of Dispersed Iron-Based Additives in Coal Liquefaction" *Am. Chem. Soc. Div. Fuel Chem. Prepr.* **1993**, *38*(1), 107.

25. Lee, T. L.; Pradhan, V. R.; Stalzer, R. H.; Comolli, A. G. "Catalytic Multi-Stage Liquefaction of Coal" U.S. DOE Coal Liquefaction and Gas Conversion Contractor's Review Conference, Sept. 27-29, 1993, Pittsburgh, PA.

26. Comolli, A. G.; Lee, L. K.; Pradhan, V. R.; Stalzer "The Direct Liquefaction Proof-of Concept Programs Runs POC-1 and POC-2" U.S. DOE Coal Liquefaction and Gas Conversion Contractor's Review Conference, Sept. 7-8, 1994, Pittsburgh, PA.

27. Comolli, A. G.; Pradhan, V. R.; Lee, T. L. K.; Karolkiewicz, W. F.; Popper, G. "Direct Liquefaction Proof-of-Concept Program, Topical Report Bench Run O3 (227-93)", DE/92148/TOP05, December 1996.

28. HTI draft report on Run PB-O5 (227-97) "Evaluation of An All-Dispersed Slurry Catalyst for Direct Liquefaction and Combined Processing of a Bituminous Illinois No. 6 Coal with Organic Waste Materials", unpublished

29. Standard Test Method for Thermal Stability of Aviation Turbine Fuels (JFTOT Procedure) ASTM D3241-77.

30. Stuntz, G. F. "Premium Products from Direct Coal Liquefaction", presented at the Alternate Energy '91 Symposium, April 16-19, 1991, Scottsdale, AZ.

31. Zhou, P-Z.; Rao, S. N. "Assessment of Coal Liquids as Refinery Feedstocks" prepared for U.S. DOE by Burns and Roe Services, Contract DE-AC22-89PC88400, Subtask 43.01, February, 1992.

32. Edwards, T.; Harrison, W. E.; Schobert, H. H. "Properties and Producibility of Advanced Jet Fuels", 33rd AIAA/ASME/SAE/ASEE Joint Propulsion Conference & Exhibit, July 6-9, 1997, Seattle, Washington.

33. Standard Specification for Aviation Turbine Fuels ASTM D 1655-97 The Annual Book of ASTM Standards.

34. Miknis, F. P. "Coal Liquefaction Process Streams Characterization and Evaluation - Solid State NMR Characterization of Coal Liquefaction Products, Topical Report", DOE/PC 89883-36, November 1991.

TABLE 1

BACKGROUND INFORMATION FOR NET PRODUCT SAMPLES

Sample ID	Plant	Feed Coal, Mine/Seam	Process Description			Yield C_4-524°C Distillate, wt% MAF coal	Laboratory
			Reactor Configuration	Reactor Temperatures, °C	Catalyst		
259 G	Wilsonville	Ireland/ Pittsburgh (cleaned)	catalytic/catalytic	441/421	Shell 324 (Ni/Mo/Al)	73.7	Conoco(a)
260 D	Wilsonville	Black Thunder/ Wyodak and Anderson	catalytic/thermal	421/412	Shell 324 (Ni/Mo/Al)	59.8	Conoco(a)
CC-15	HTI	Black Thunder/ Wyodak and Anderson	thermal/catalytic	427/413	Shell 317 (Ni/Mo/Al)	60.5	NIPER(b)
CMSL-2	HTI	Burning Star No. 2/ Illinois No. 6	catalytic/catalytic	400-414/424-433	Shell 317 (Ni/Mo/Al)	75.9	NIPER(b)
POC-1	HTI	Crown II/ Illinois No. 6	catalytic/catalytic	412/440	Akzo AO60, 1/16"	70 - 74	Conoco(a)
POC-2	HTI	Black Thunder/ Wyodak and Anderson	catalytic/catalytic	430/443	Akzo AO60, 1/16"	58 - 66	Conoco(a)
PBO3-6,7,8	HTI	Black Thunder/ Wyodak and Anderson	catalytic/catalytic	441/449	dispersed Fe and Mo	57.4	Caleb Brett(c)
PBO3-9,10,11	HTI	Black Thunder/ Wyodak and Anderson	catalytic/catalytic	441/449	dispersed Fe and Mo	55.4	Caleb Brett(c)
PBO5-22-25	HTI	50% Crown II/ Illinois No. 6; 50 % Hondo Petroleum Resid	catalytic/catalytic	448/460	dispersed Fe, Mo, and P	89.0	Caleb Brett(c)

(a) Conoco Inc., Research and Engineering Dept., Ponca City, OK
(b) IIT Research Institute, National Institute for Petroleum and Energy Research, Bartlesville, OK
(c) Inchcape Testing Services Caleb Brett Laboratory, Houston, TX

TABLE 2

DISTILLATION CUTS OF NET PRODUCTS, °C

Equivalent Petroleum Cut	259G	260D	CC-15	CMSL-2	POC-1	POC-2	PBO3-6,7,8	PBO3-9,10,11	PBO5-22-25
naphtha/gasoline							<21	<21	<21
					<82	<82	21-82	21-82	21-82
	<193	<193	<193	<177	82-177	82-177	82-177	82-177	82-177
jet fuel	193-266	193-266	193-266	177-204	177-204	177-204	177-204	177-204	177-204
				204-288	204-260	204-260	204-288	204-288	204-288
					260-288	260-288			
diesel fuel/heating fuel	>266	266-343	266-337		288-343	288-343	288-343	288-343	288-343
heavy heating oil		>343	>337	>288	>343	>343	>343	>343	>343

TABLE 3

TEST METHODS USED FOR PETROLEUM INSPECTION TESTS OF JET FUEL CUTS

Test and Units Reported	ASTM Method A	ASTM Method B	Method C	Method D or Reference
gravity, API	D1298	D4052	2-API	
gravity, specific, 60/60	D4052	D4502	2-API	
S, tot, wt %	D3120	D4294		
mercaptan S, ppm	D3227		UOP163	
C, wt %	D5291		Leco CHNS -932	
H, wt %	D5291		Leco CHNS -932	
N, wt %	D4629			
basic N, wt %			UOP269	
refractive index	D1218			
bromine number, g/100g	D1159			
viscosity, csT at 40 °C	D445			
viscosity, csT at 100 °C	D445			
viscosity, csT at -20 °C	D445			
aniline point, °F	D611			
freeze pnt, °F	D2386			
cloud pnt, °F	D2500			
smoke pnt, mm	D1322			
paraffins, vol %	D5134		HC22; Analytical Controls Method	GC-PONA
naphthenes, vol %	D5134		HC22; Analytical Controls Method	GC-PONA
aromatics, vol %	D5134		HC22; Analytical Controls Method	GC-PONA
olefins, vol %	D1319			
Reid vapor pressure, psi	D5191			
vapor pressure, psi	D323			
thermal stability (JFTOT)	D3241			
copper strip corrosion	D130			
existent gum test (washed), mg/100mL	D381			
existent gum test (unwashed), mg/100mL	D323			
oxidation stability, min	D525			
oxidation stability, mg/100mL	D2274			
acidity, mg KOH/g	D3242	D974	D 664	
heat of combustion, Btu/lb	D2382	D4529	D240	D1 405
flash pnt, °F	D56	D93		
cetane index	Calc. D976			
cetane number	D613			
naphthalenes, v%	D1840			
luminometer number	D1740			
tube rating	D3241			
research octane number	D2699		Phillips Tech Svc. KEAS	
motor octane number	D2700		Phillips Tech Svc. KEAS	
Distillation - volume % recovery @ °F	D86			
phenolic -OH meq/g				Reference 21
oxygen content, wt% phenolic				Reference 21
oxygen content, wt% total			by difference	
proton distribution				Reference 21

TABLE 4
SAMPLE PROPERTIES

Sample	Jet A-1 Spec[32]	259G	260D	CC-15	CMSL-2		POC-1			POC-2			PBO3-6,7,8		PBO3-9,10,11		PBO5, 22-25	
bp of Cut, °C		193-266	193-266	193-266	177-204	204-288	177-204	204-260	260-288	177-204	204-260	260-288	177-204	204-288	177-204	204-288	177-204	204-288
vol % of crude		31.04	18.63				8.26	21.39	14.73	9.18	21.53	13.55	8.65	25.84	10.16	30.87	9.98	31.3
wt % of crude		31.39	18.95	33.4	5.6	35.2	8.16	21.93	15.51	9.04	22.03	14.3	8.74	27.52	10.35	32.37	9.99	32.68
gravity, API	37-51	25.90	21.3	27.5[C]	35.1[C]	27.6[C]	34.2[B]	28.2[B]	23.9[B]	36.3[B]	29.9[B]	25[B]	36.2[B]	27.5[B]	21.1[B]	16.8[B]	33.7[B]	26.9[B]
gravity, specific, 60/60		0.8990	0.9260	0.8899[B]	0.8492[B]	0.8892[B]	0.8542[A]	0.886[A]	0.9103[A]	0.8435[A]	0.8765[A]	0.904[A]	0.8437[A]	0.8898[A]	0.9268[A]	0.954[A]	0.8565[B]	0.8932[B]
S, tot, wt %	0.3 max	0.04	0.04	0.03[A]	0.01[A]	0.01[A]	0.036[B]	0.03[B]	0.022[B]	0.003[B]	0.002[B]	0.003[B]	0.03[B]	0.02[B]	0.17[B]	0.12[B]	0.18[B]	0.47[B]
mercaptan S, ppm	30 max	30	85	45[A]	19[C]		70[A,C]	40[A,C]	37[A,C]	<10[A,C]	<10[A,C]		16[C]	17[C]	597[C]	126[C]	214[B]	262[B]
C, wt %		87.00	85.8	87.12[A]	86.78[A]	87.48[A]	86.7[C]	87.3[C]	87.7[C]	86.6[C]	87[C]	87.4[C]	86.38[A]	87.79[A]	81.77[A]	83.85[A]	84.64[A]	85.48[a]
H, wt %		11.50	10.6	11.77[A]	12.72[A]	12.27[A]	12.64[C]	12.13[C]	11.9[C]	13.16[C]	12.74[C]	12.38[C]	13.17[A]	12.14[A]	10.54[A]	10.15[A]	11.83[A]	11.26[A]
N, wt %		<0.1	0.3	0.33	0.03	0.03	0.059	0.066	0.55	0.002	0.01	0.008	0.006	0.02	0.589	0.12	0.57	0.74
basic N, wt %		0.09	0.219	0.274	0.023	0.029		0.051	0.037		0.009	0.006		0.002		0.597		0.532
refractive index		1.4774	1.4850	1.49196														
bromine number, g/100g		8.90	25	5.08	3.00	1.94												
viscosity, cSt at 40 °C						2.503	1.065	1.914		1.07	2.042	3.79		2.203		4.216		2.50
viscosity, cSt at 100 °C					0.6653	1.056		0.81	1.3		0.754	1.35	0.569	0.952	0.750	1.199	0.664	0.969
viscosity, cSt at -20 °C	8 max	1.75	18.94	10.80	4.683		4.35	10.71	3.71	4.12	10.22		3.832	12.65	12.42	73.47*	6.46	19.83
aniline point, °C		23.30	17.2	21.9				28.3	33.3		40.6	43.9		32.7		-7.5		33.6
freeze pnt, °C	-53.5max	-53.50	too dark	-24.4	-72.8		<-51.1	-48.3		<-51.1	<-51.1		-60	-41.6	-48.8	-28.3	-56	-31.5
cloud pnt, °C					<-51	<-51												
smoke pnt, mm	25 min	10.80	9.8	10.9	15.6		13.7	11.8		17.7	11.7		18	11	13	9	36	10
paraffins, vol %			42.0	9.6[A,C]	7.5[A,C]	7.5[A,C]	6.57[C]	0.94[C]	0.39[C]	8.24[C]	0.26[C]		13.13[D]	11.52[D]	21.46[D]	13.95[D]	32.47[D]	22.73[D]
naphthenes, vol %			4.94	43.1[A,C]	61.3[A,C]	53.0[A,C]	18.22[C]	0.36[C]	0.13[C]	20.41[C]	0.59[C]		60.58[D]	39.1[D]	11.83[D]	20.97[D]	18.66[D]	16.87[D]
aromatics, vol %	25 max	44.0	50.0	41.4[A,C]	28.4[A,C]	37.5[A,C]	31.19[C]	1.37[C]	0[C]	21.19[C]	0.79[C]		23.89[D]	35.88[D]	57.51[D]	60.68[D]	42.07[D]	51.8[D]
olefins, vol %		3.0	3.0	5.8	2.8	2.0		4		1	1.00		2.40	13.5	9.2	4.4	6.8	8.6
Reid vapor pressure, psi				<0.01	0.02		0.12	0.12		0.07	0.15							
vapor pressure, psi		0.2	0										0.2		0.2		0.1	
thermal stability (JFTOT)	25	failed**		failed			fail/4	fail/4		fail/4	too foamy							
copper strip corrosion	1 max	1A	1A	1A	1A	1A	1A	1A	1A	1A	1A	1A	4A	3A	3A	1A	1A	1A
existent gum test (washed), mg/100 mL	7 max	40.60	83	bp too high	6.4	52.6	16.8	9.4	7.6	1.2	3.6	6.8	6	8	63	40	21	29
existent gum test (unwashed), mg/100 mL		69.0	90.8															
oxidation stability, min					1440		960	960	960	960	960	960	>240		>240		>240	
oxidation stability, mg/100 mL						1												
acidity, mg KOH/g	0.1 max	0.05	0.50	0.04[A]	0.01[A]	0.01[A]	0.01[B]	<0.01[B]		0.011[B]	<0.01[B]		0.08[B]	0.03[B]	0.70[C]	0.74[B]		
heat of combustion, MJ/kg	42.8 min	42.1	42.0	41.7[A]	42.8[C]		42.1[B]	41.9[B]		42.7[B]	42.4[B]		42.6[D]	41.7[D]	42.2[D]	42.3[D]	43.1[D]	42.6[D]
flash pnt, °C	38 min	76.1	188	83[A,B]	50[A,B]	94.5[A,B]	56.6[A,B]	82.2[A,B]	121[A,B]	54.4[A,B]	82.2[A,B]	115.6[A,B]	57.2[A]	90.6[A]	65.6[A]	>93.3[A]	57.7[A]	93.3[A]
cetane index		22.9			20.8	32.7	20.57	26.9	31.9	21.8	29.3							
cetane number													29.9	31.6	<18.3	<18.3	19.4	19.6
naphthalenes, vol %	3 max			4.23	0.48		1	2.6		0.11	0.56		0.36	5.11	6.34	14.92	18.66	7.02
luminometer number	45 min				27.3		27.2	22		38	21.8		42	23	33	22	36	22
tube rating													4.0	>4.0	4.0	4.0		
research octane number							65.24[C]			52.66[C]			54.7[A]		106.6[A]		92.0[A]	
motor octane number							62.83[C]			50.02[C]			52.1[A]		91.2[A]		79.2[A]	

Uppercase letter superscripts refer to test methods, see Table 3

*value questionable
**excessive foaming

TABLE 4
SAMPLE PROPERTIES (continued)

Sample	Jet A-1 Spec[33]	259C	260D	CC-15	CMSL-2		POC-1			POC-2			PBO3-6,7,8		PBO3-9,10,11		PBO5, 22-25	
BP of Cut, °C		193-266	193-266	193-266	177-204	204-288	177-204	204-260	260-288	177-204	204-260	260-288	177-204	204-288	177-204	204-288	177-204	204-288
Distillation - volume % recovery @°F																		
IBP		142.5		408.2	322.7	434.8	348.8	400	458.2	348.6	400	508	356	428	351	412	350	425
1			380															
5		429.6	401	425.6	362.1	457.7	368.2	430	458.2	359.2	429	511	360	436	360	433	355	436
10	401	427.2	414	428.1	365.9	461.6	369.1	424	516.5	361.2	424	511	361	442	361	439	355	438
20		433.2	434	433	368.2	466.3	370.4	434	515.8	362.3	434	507	361	446	365	444	357	442
30		421.7	449	438.7	370	473.5	371.4	438	518.9	363.3	438	510	363	451	367	450	358	446
40		433.7	457	442.7	372.5	480.5	372.9	441	518.5	365.1	441	512	365	457	369	457	360	451
50		440.7	468	448.1	375.2	486.6	374.7	445	520.1	366.9	445	512	366	464	370	462	362	458
60		443.4	476	454.4	378.1	494.9	376.8	449	522.5	368.7	448	511.8	368	471	372	471	364	465
70		447.8	483	461.6	381.3	504.5	379.2	456	524.8	371.4	456	512.6	371	480	376	480	367	475
80		457.7	491	470.4	385.3	513.3	382.2	461	528.9	374.5	461	517.6	374	491	378	484	371	486
90		471.5	499	478.9	391.8	526.1	386.7	469	535.6	379.2	469	522.1	378	503	383	504	377	500
95		483.4	509	486.8	397.2	535.2	390.3	484.3	541.4	382.8	480	528.2	382	508	388	514	382	514
99			536															
end pnt, vol %	572	98.5																
end pnt T, F		505.9		507.9	401.5	540.5	400.8	490	555.2	393.9	490	535.8	401	524	403	532	392	525
recovery %		98.7		99.5	97.1	97.7	98.5	98.2	98.1	99.1	98.0	98.2	99.0	99.0	99.0	99	98.7	98.4
residue %	1.5 max	1.0		0	0.9	1.3							1.0	0.9	0.5	0.5	1.3	0.8
total recovery %		99.7													99.5	99.5		99.2
wt% raffinate of feed					98	99												
phenolic -OH meq/g		0.25	0.92	0.24	ND	ND												
oxygen content, wt % phenolic		0.4	1.47	0.38														
oxygen content, wt % total		1.4	3.3	0.75	0.46													
proton distribution																		
cond arom		2.0	6.6	3.1	1.3	1.3												
uncond arom		6.8	10.4	6.8	5	5.0												
cyclic alpha		8.0	8.3	10.7	5.7	7.9												
alkyl alpha		8.6	10.1	9.7	6.2	8.0												
cyclic beta		22.8	18.4	20.6	22	22.1												
alkyl beta		29.7	27.4	28.1	31.4	30.6												
gamma		22.0	18.9	20.9	28.3	25.1												

ND = none detected

TABLE 5

JET FUEL AND RAFFINATE ANALYSES

Sample Jet A-1 Spec	W260D	Caustic washed W260D	HRI CC-15	Caustic washed CC-15	HRI CMSL-2	Caustic washed CMSL-2
BP of Cut, °C	193-226	193-226	193-226	193-226	177-204	177-204
vol % of crude	18.63					
wt % of crude	18.95		33.4		5.6	
gravity, API	21.3		27.5(d)	27.8(d)	35.1(d)	35.3(d)
gravity, specific, 60/60	0.9260		0.8899	0.8882	0.8492	0.8484
S, tot, wt %	0.04		0.03	<0.01	0.01	0.01
mercaptan S	0.0085, wt%		45.2 ppm	<0.1 ppm	19	6
C, wt %	85.8		87.12	87.75	86.78	86.68
H, wt %	10.6		11.77	11.68	12.72	13.08
N, wt %	0.3		0.33	0.33	0.03	0.02
basic N, wt %	0.219		0.274	0.264	0.023	0.023
refractive index	1.4850		1.49196	1.49072		
bromine number, g/100g	25		5.08	2.69	3.00	2.71
viscosity, cSt at 210F					0.6653	0.6741
viscosity, cSt at -20C	18.94		10.80	9.665	4.683	4.359
aniline point, °F	63		71.5	75.2		
freeze pnt, °C	too dark		-12	-13	-99	-95
cloud pnt, °F					<-60	<-60
smoke pnt, mm	9.8		10.9	11.6	15.6	15.4
paraffins, vol %	47.0(a)		9.6	9.1	7.5	8.0
naphthenes, vol %	4.94		43.1	46	61.3	61.5
aromatics, vol %	50.0		41.4	41.9	28.4	27.8
olefins, vol %	3.0		5.8	3.0	2.8	2.5
Reid vapor pressure, psi	0.0		<0.01	<0.01	0.02	<0.01
thermal stability (JFTOT)			failed	failed		
copper strip corrosion	1A		1A	1A	1A	1A
existent gum test (washed), mg/100 mL	83.0		(b)	(b)	6.4	6.2
existent gum test (unwashed), mg/100 mL	90.8					
oxidation stability, min					1440	720
acidity, mg KOH/g	0.50		0.04	0.01	0.01	<0.01
heat of combustion, MJ/kg	42, calc.		41.676, net		42.8, net	42.8, net
flash pnt, C	188		83	82	50	57
cetane index					20.8	
naphthalenes, v%			4.23	3.74	0.48	0.32
wt% raffinate of feed		92.7		92.06	98	95.4
phenolic -OH meq/g	0.92	0.07	0.24 (e)	(c)	(c)	(c)
oxygen content, wt% phenolic	1.47		0.38			
oxygen content, wt% total	3.3		0.75	0.23	0.46	
proton distribution						
cond arom	6.6	6.5	3.1	3.2	1.3	0.6
uncond arom	10.4	8.3	6.8	6.4	5	4.8
cyclic alpha	8.3	6	10.7	11.3	5.7	5.8
alkyl alpha	10.1	7.7	9.7	10.0	6.2	6.4
cyclic beta	18.4	21.4	20.6	21.2	22	23.7
alkyl beta	27.4	28.8	28.1	27.6	31.4	30.9
gamma	18.9	21.2	20.9	20.4	28.3	27.7

a Includes naphthenes
b Boiling point too high
c Amine observed, no phenolic -OH detected
d Calculated
e Amines observed; probably contributed to phenolic -OH concentration

TABLE 6

API GRAVITY, DENSITY, AND HEAT OF COMBUSTION

Sample	Jet A-1 Spec[33]	259G	260D	CC-15	CMSL-2	POC-1		POC-2		PBO3-6,7,8		PBO3-9,10,11		PBO5, 22-25	
BP of Cut, °C		193-266	193-266	193-266	177-204	177-204	204-260	177-204	204-260	177-204	204-288	177-204	204-288	177-204	204-288
gravity, API	37-51	25.90	21.3	27.5	35.1	34.2	28.2	36.3	29.9	36.2	27.5	21.1	16.8	33.7	26.9
gravity, specific, 60/60	.7753 - .8397 (a)	0.8990	0.9260	0.8899	0.8492	0.8542	0.886	0.8435	0.8765	0.8437	0.8898	0.9268	0.954	0.8565	0.8932
density, kg/L @ 60 °F (b)	.7746 - .8389	0.8981	0.9251	0.8891	0.8484	0.8534	0.8852	0.8427	0.8757	0.8429	0.889	0.9259	0.9531	0.8557	0.8924
heat of combustion, MJ/kg	42.8	42.1	42.0	41.7	42.8	42.1	41.9	42.7	42.4	42.6	41.7	42.2	42.3	43.1	42.6
heat of combustion, MJ/L(c)	33.2 - 35.9	37.9	37.8	37.1	36.3	35.9	37.1	36	37.1	35.9	37	39.1	40.3	36.9	38

a Values calculated from ASTM Jet A-1 specifications for API gravity using:

$$API_{grav} = \left(\frac{141.5}{\text{spgr } 60/60}\right) - 131.5$$

b Calculated from:

$$\text{specific grav } 60/60 = \frac{\text{mass of sample at } 60\,°F/L}{\text{mass of water at } 60\,°F/L}$$

mass of water at 60 °F = 0.9990499

c Calculated from density (kg/L) and heat of combustion (MJ/kg)

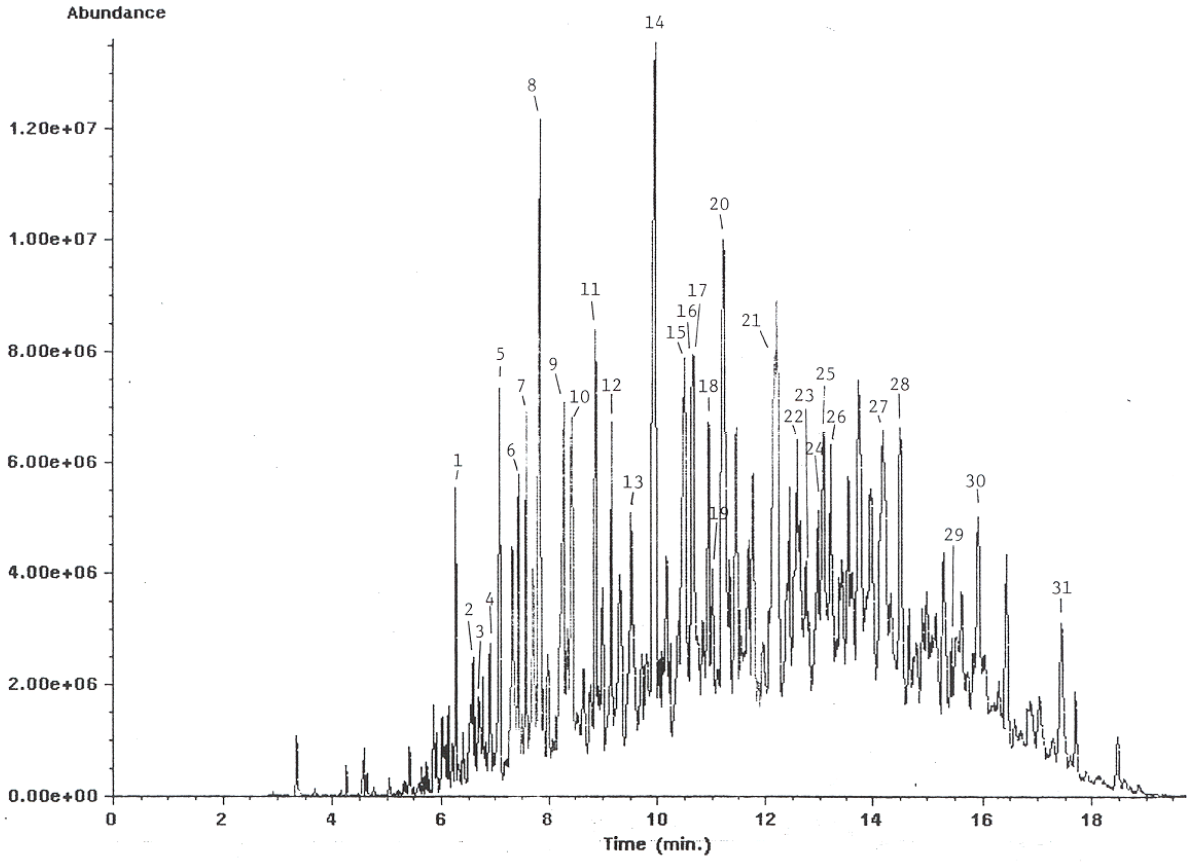

Figure 1. Total Ion Chromatogram, Jet Fuel Fraction, Wilsonville Run 259G Product. (See key following this figure.)

KEY TO PEAK IDENTIFICATIONS
Figure 1

Peak No.	Identification
1	trans-Decalin
2	Methylindan
3	n-Undecane
4	cis-Decalin
5	Methyldecalin
6	Methylindan
7	Methylindan
8	Tetralin
9	Naphthalene
10	C_2-Indan
11	Methyltetralin
12	C_2-Indan
13	C_2-Indan
14	Methyltetralin
15	Methyltetralin
16	n-Tridecane
17	Methylnaphthalene
18	Bicyclohexyl
19	Methylnaphthalene
20	C_2-Tetralin
21	Ethyltetralin
22	Tetrahydroacenaphthene
23	unknown
24	C_2-Tetralin
25	C_2-Tetralin
26	n-Tetradecane
27	Butyltetralin
28	C_3Tetralin?
29	Acenaphthene
30	n-Pentadecane
31	Butyltetralin

NOTES: Identifications based on search of Wiley/NBS Library of mass spectra. C_x refers to alkyl substituents of x carbon atoms. Search results may misidentify isomers.

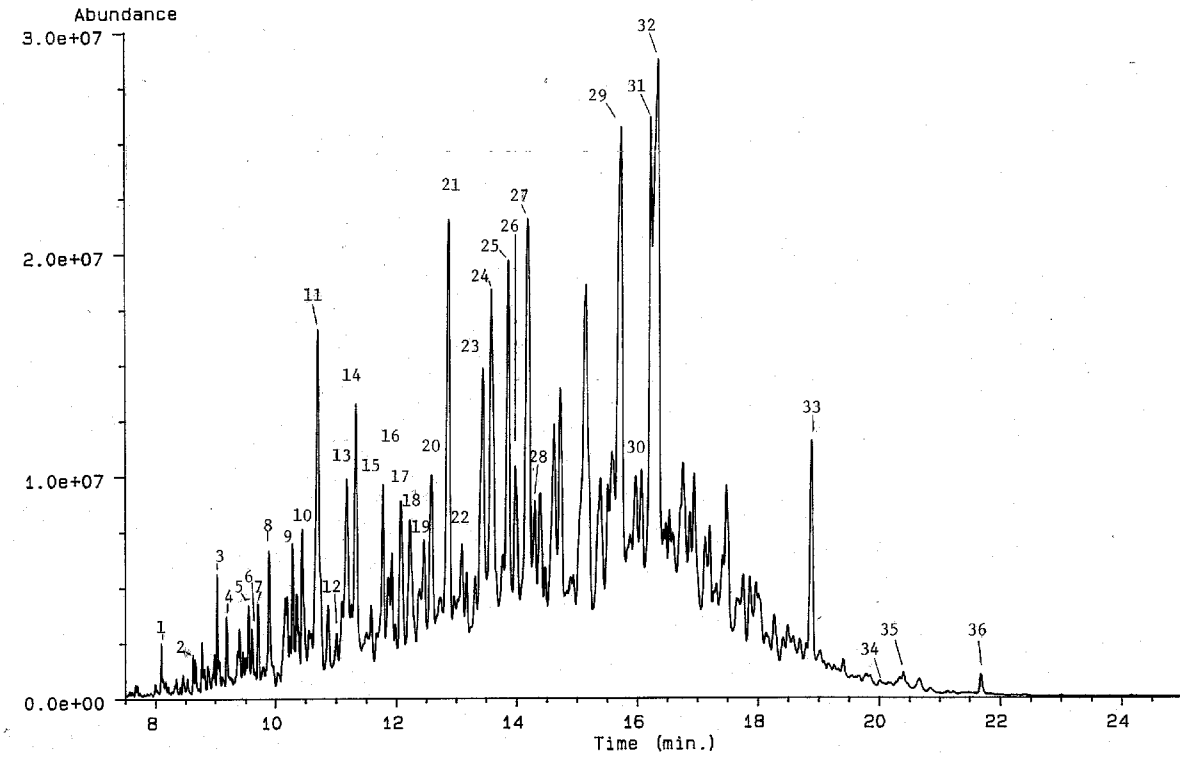

Figure 2. Total Ion Chromatogram, Jet Fuel Fraction, Wilsonville Run 260D Product. (See key following this Figure.)

KEY TO PEAK IDENTIFICATIONS
Figure 2

Peak No.	Identification
1	Hexahydroindan
2	Indan
3	Decalin
4	O-Cresol
5	Methylindan
6	n-Undecane
7	Methyldecalin
8	Methyldecalin
9	Methylindan
10	Methylindan
11	Tetralin
12	Methyldecalin
13	Naphthalene?
14	n-Dodecane
15	Methyltetralin
16	C_3-Phenol
17	Methyltetralin
18	C_5-Cyclohexane
19	C_2-Indan
20	C_3-Phenol
21	Methyltetralin
22	C_2-Indan
23	Methyltetralin
24	n-Tridecane
25	Bicyclohexyl
26	Methylnaphthalene
27	Methylnaphthalene
28	C_3-Indan
29	Biphenyl
30	C_2-Tetralin
31	n-Tetradecane
32	Diphenyl Ether
33	n-Pentadecane
34	Octahydroanthracene
35	C_4-Tetralin
36	n-Hexadecane

NOTES: Identifications based on search of Wiley/NBS Library of mass spectra, C_x refers to alkyl substituents of x carbon atoms. Search results may misidentify isomers.